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Tsallis Statistics: Averages and a Physical Interpretation of the Lagrange Multiplier β

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ABSTRACT

Tsallis has proposed a generalisation of the standard entropy, which has since been applied to a variety of physical systems. In the canonical ensemble approach that is mostly used, average energy is given by an unnromalised, or normalised, q-expectation value. A Lagrange multiplier β enforces the energy constraint whose physical interpretation, however, is lacking. Here, we use a microcanonical ensemble approach and find that consistency requires that only normalised q-expectation values are to be used. We then present a physical interpretation of β, relating it to a physical temperature. We derive this interpretation by a different method also.

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1. Tsallis has proposed [1] a one parameter generalisation of the standard Boltzmann-Gibbs entropy. It is given by

$$S_q = \frac{\sum p_i^q - 1}{1 - q} \tag{1}$$

where p_i is the probability that the system is in a state labelled by i, the sum, here and in the following, runs over all the allowed states, and the parameter q is a real number. We have set the Boltzmann constant k equal to unity. In the limit $q \to 1$, $S_q = -\sum p_i ln p_i$, thus reducing to the standard Boltzmann-Gibbs entropy. The statistical mechanics that follows from the entropy S_q, referred to here as Tsallis statistics, is rich in applications and has been studied extensively. It retains the standard thermodynamical structure, leads to power-law distributions as opposed to the exponential ones that follow from the standard statistical mechanics, and has been applied to a variety of physical systems. See [2, 3] for a thorough discussion, and [4] for an exhaustive list of references.

Mostly, in these applications, a canonical ensemble approach is used [1, 5]. The entropy S_q is extremised subject to the constraint $\sum p_i = 1$, and an average energy constraint (equation (2) below), obtaining thus the probability distribution p_i. Various thermodynamical quantities are then calculated by standard methods[1].

The averages can be taken to be given by unnormalised, or normalised, q-expectation values. Calculations are simpler with the former choice, whereas the later choice has all desireable properties. Also, various quantities calculated using these two choices, although not equal to each other, can be related by a set of formulae. Therefore, both choices have often been used. See [5] and references therein for a detailed discussion. The average energy constraint is then enforced through a Lagrange multiplier, β. In the standard statistical mechanics, β is the inverse of the temperature which can be physically measured. To the best of our knowledge, a similar physical interpretation of β in Tsallis statistics is still lacking. (However, see the Note at the end of the paper.)

In the present letter, we use the microcanonical ensemble approach [1] and calculate the temperature and specific heat using the entropy S_q. For

[1] Since the standard thermodynamical structure is preserved, such quantities can be calculated using the standard formulae [2]. However, they are mathematical constructs only, which may or may not have a physical meaning.

classical ideal gas, various thermodynamical quantities have been calculated in [6, 7] using the canonical ensemble approach. Upon comparing the specific heats obtained in the microcanonical and the canonical ensemble approaches, we find that these two approaches can be equivalent, and various quantities calculated in these two approaches can be equal to each other, only if the average is given by normalised q-expectation value, and not by unnormalised one.

We then present a physical interpretation of the temperature calculated in the microcanonical ensemble. Comparing then with the canonical ensemble results of [7], we obtain a physical interpretation of the Lagrange multiplier β. Interestingly, the same interpretation can be derived by a simple refinement of the Gibbsian argument of Plastino and Plastino [8]. We present this derivation also.

The plan of the paper is as follows. We first give the relevant details [5] and results [6, 7] of the canonical ensemble approach. We then present our results, and close with a few comments.

2. In the canonical ensemble approach, the entropy S_q is extremised subject to the constraint $\sum p_i = 1$, and an average energy constraint. One thus obtains the probability distribution p_i, and calculates the physical quantities by standard methods. We briefly present here the relevant aspects. We follow [5], where more details can be found.

The average energy U of the system can be taken to be given by unnormalised, or normalised, q-expectation value as follows:

$$U_2 = \sum p_i^q \epsilon_i \ , \quad \text{or} \quad U_3 = \frac{\sum p_i^q \epsilon_i}{\sum p_i^q} \ , \tag{2}$$

where ϵ_i is the i^{th} state energy. Here and in the following, the subscript 2 (3) indicates that the averages are given by unnormalised (normalised) q-expectation values. Extremising S_q, with the average energy given by U_2 (U_3) in (2), gives

$$p_{i2} = \frac{a_{i2}}{Z_2} \ , \quad a_{i2} = (1 - \beta_2 (1-q) \epsilon_i)^{\frac{1}{1-q}} \tag{3}$$

$$p_{i3} = \frac{a_{i3}}{Z_3} \ , \quad a_{i3} = \left(1 - \frac{\beta_3 (1-q)(\epsilon_i - U_3)}{Y_3} \right)^{\frac{1}{1-q}} \ , \tag{4}$$

where $Z_{2(3)} = \sum a_{i2(3)}$, and β_2 (β_3) is the Lagrange multiplier for U_2 (U_3). It

also follows that

$$Y_2 \equiv \sum p_{i2}^q = Z_2^{1-q} + \beta_2 (1-q) U_2 \ , \quad Y_3 \equiv \sum p_{i3}^q = Y_3 = Z_3^{1-q} \ .$$

3. Consider systems whose standard Boltzmann-Gibbs, namely $q = 1$, partition function is of the form

$$Z_{BG} \propto l^a \beta^{-a} \tag{5}$$

where a is a dimensionless parameter, l is a characteristic length, and β is the inverse temperature. For example, for a d-dimensional classical ideal gas with N particles and volume V, $a = \frac{dN}{2}$ and $l \propto V^{\frac{1}{d}}$. For classical ideal gas, the above formalism has been applied, and various quantities such as energy, specific heat, etc. have been calculated in [6, 7]. The average energies U_2, U_3 and the specific heats $\mathcal{C}_2, \mathcal{C}_3$ are given by [2]

$$\beta_2 U_2 = \frac{a Y_2}{1 + (1-q) a} \ , \qquad \mathcal{C}_2 = a Y_2 \tag{6}$$

$$\beta_3 U_3 = a Y_3 \ , \qquad \mathcal{C}_3 = \frac{a Y_3}{1 - (1-q) a} \ . \tag{7}$$

Note that the specific heats $\mathcal{C}_2$ and $\mathcal{C}_3$ are not equal to each other, and even have qualitatively different behaviour: $\mathcal{C}_2$ is always positive since $Y_2 \equiv \sum p_{i2}^q$ is always positive, whereas $\mathcal{C}_3$ becomes negative when $(1-q)a > 1$. Explicit expressions for Y_2 and Y_3 can be found in [6, 7], but are not needed here.

4. However, one can also use the microcanonical ensemble approach [1]. For a given energy E_{mc} of the system, the entropy is extremised subject only to the constraint $\sum p_{i(mc)} = 1$. The subscript mc, here and in the following, indicates that the microcanonical ensemble approach is used. Note that no averaging of the energy is involved in this approach and, hence, no choice is made.

The entropy S_q is extremised in the case of equiprobability, *i.e.* when all the probabilities are equal, with the extremum being a maximum (minimum) if $q > 0$ ($q < 0$) [1]. Thus, if W is the number of allowed states then

$$p_{i(mc)} = \frac{1}{W} \quad \text{and, hence,} \quad S_q = \frac{W^{1-q} - 1}{1 - q} \ . \tag{8}$$

[2] As mentioned in section **1**, $(\beta_2, U_2, \mathcal{C}_2, \cdots)$ and $(\beta_3, U_3, \mathcal{C}_3, \cdots)$ can be related to each other by a set of formulae [9].

Since the standard thermodynamical structure is preserved [2], the inverse temperature β_{mc} and the specific heat $\mathcal{C}_{mc}$ can be calculated using the standard formulae:

$$\beta_{mc} \equiv \frac{\partial S_q}{\partial E_{mc}} = \beta_* Y_{mc} \tag{9}$$

$$\mathcal{C}_{mc} \equiv -\beta_{mc}^2 \left(\frac{\partial^2 S_q}{\partial E_{mc}^2} \right)^{-1} = \frac{c_* Y_{mc}}{1 - (1-q) c_*} \,, \tag{10}$$

where we have defined $Y_{mc} = \sum p_{i(mc)}^q = W^{1-q}$,

$$\beta_* = \frac{\partial lnW}{\partial E_{mc}} \,, \quad \text{and} \quad c_* = -\beta_*^2 \left(\frac{\partial^2 lnW}{\partial E_{mc}^2} \right)^{-1} \,. \tag{11}$$

For systems whose $q = 1$ partition function is given by (5), we have

$$W \propto l^a E_{mc}^a \quad \text{and, hence,} \quad \beta_* = \frac{a}{E_{mc}} \,, \quad \text{and} \quad c_* = a \,. \tag{12}$$

Equations (9) and (10) then give

$$\beta_{mc} E_{mc} = a Y_{mc} \,, \quad \mathcal{C}_{mc} = \frac{a Y_{mc}}{1 - (1-q) a} \,. \tag{13}$$

5. For systems whose $q = 1$ partition function is given by (5), we now have expressions (6), (7), and (13) for energy and specific heat, obtained using the canonical [6, 7] and the microcanonical ensemble approach. The canonical ensemble approach involves an averaging of the energy, and the expressions (6) ((7)) are for the case where the average is given by unnormalised (normalised) q-expectation value. However, in the microcanonical ensemble approach, no averaging of energy is involved and, hence, no choice is made.

Let us now compare the specific heats. The specific heats given by (7) and (13) are identical, upto factors involving Y_3 and Y_{mc}, and differ distinctly from that given by (6). For example, the specific heat given by (6) is always positive, whereas the specific heats given by (7) and (13) become negative when $(1-q)a > 1$. Therefore, it follows that the microcanonical and the canonical ensemble approaches can be equivalent, and various quantities calculated in these two approaches can be equal to each other, only if the

average is given by normalised q-expectation value, and not by unnormalised one.

6. From now on, we assume that the averages are given by normalised q-expectation values only. Therefore, energy and specific heat in the canonical ensemble approach are given by (7). We now present a physical interpretation of β_* in (11) and, thus, also of β_{mc} and β_3.

Consider a system obeying Tsallis statistics, with q positive but otherwise arbitrary, with energy E and number of allowed states $W(E)$, and enclosed within a container with which it can exchange energy only. Together, let them be isolated. Thus, if E_c is the energy of the container then the total energy $E_{tot} = E + E_c$ is fixed. Let the container be choosen to obey the standard Boltzmann-Gibbs statistics, namely Tsallis statistics with $q = 1$. Therefore, if $W_c(E_c)$ is the number of allowed states of the container, then

$$\beta_{phys} = \frac{\partial lnW_c}{\partial E_c} \tag{14}$$

is the inverse of its temperature, which can be physically measured.

We would like to find the values E of the system, and $E_c = E_{tot} - E$ of the container, at which the (system + container) is in equilibrium. But the analysis of such a composite system, where the constituent systems have different values of q, is highly nontrivial and is still an open problem[3]. Nevertheless, it is reasonable to expect that **(i)** the entropy of the composite system is extremised in the case of equiprobability; **(ii)** the extremum is a maximum, at least in the case where the q's of the constituent systems are all positive; and **(iii)** the maximum is a monotonically increasing function of the total number of allowed states of the composite system.

Although we are unable to justify these properties rigorously, they appear to be physically reasonable, and are satisfied by any single system obeying Tsallis statistics with $q > 0$ [1], see equation (8). Hence, we assume that *any composite system, the q's of whose constituent systems are all positive, also satisfies the properties* **(i)-(iii)** *given above.* Since the entropy is extremised in equilibrium, our assumption then implies that **(i')** when a composite system is in equilibrium, the energies of its constituents will be such as to maximise the total number of states of the composite system[4]. Note that

[3] We thank the referee for emphasising this point.

[4] Alternatively, we may instead assume that *the composite system satisfies the property* **(i')** *only*, which will suffice for our purposes here.

no assumption is made, or implied, about the explicit form of the entropy of the composite system by assuming the properties **(i)-(iii)** or **(i')** for the composite system.

In the case of the (system + container) considered above, this assumption then implies that in equilibrium, the energy E of the system, and the energy $E_c = E_{tot} - E$ of the container, will be such as to maximise the total number of states of the (system + container), given by

$$W_{tot}(E_{tot}) = W(E) W_c(E_{tot} - E) \ .$$

Hence, with $E_{tot} = E + E_c$ fixed, we have that in equilibrium,

$$\frac{\partial ln W(E)}{\partial E} = \frac{\partial ln W_c(E_c)}{\partial E_c} \ . \tag{15}$$

It then follows from equations (9), (11), and (14) that

$$\beta_{phys} = \beta_* = \frac{\beta_{mc}}{Y_{mc}} \ , \tag{16}$$

which relates β_{mc} of the microcanonical ensemble approach to β_{phys}, the physical inverse temperature of the container. As clear from its derivation, the above relation is valid for any arbitrary system, whose $q = 1$ partition function is completely general.

Now, assuming the equivalence of the microcanonical and the canonical ensemble approach, we can set $E_{mc}(\beta_{mc}) = U_3(\beta_3)$. For systems considered here, whose $q = 1$ partition function is given by (5), it then follows from equations (7), (13), and (16) that

$$\frac{\beta_3}{Y_3} = \frac{\beta_{mc}}{Y_{mc}} = \beta_{phys} \ , \tag{17}$$

which relates β_3 to β_{phys}, the inverse temperature of the container, which can be physically measured. Equation (17) thus provides a physical interpretation of the Lagrange multiplier β_3 of the canonical ensemble approach.

7. The relation (17) between β_{phys} and β_3 can also be derived by another method. Plastino and Plastino have derived the probability distribution of the form given in (3), for $q < 1$, by a Gibbsian argument [8]. A simple refinement of their argument leads to the probability distribution of the form given in (4). Requiring it to be exactly identical with (4) then leads to (17).

The argument of [8] is, briefly, the following. Consider a large, but finite, heat bath obeying the standard Boltzmann-Gibbs thermodynamics. Let E_b be its energy and β_{phys} its inverse temperature, which can be physically measured. Also, let the total number of states in the energy range $(E_b \pm \frac{\Delta}{2})$ be $\eta(E_b)\Delta$. Consider now a system weakly interacting with such a heat bath. Then, the probability $p_i(\epsilon_i)$ that the system is in a state i, with energy ϵ_i, is given by

$$p_i(\epsilon_i) \propto \eta(E_b - \epsilon_i)\Delta \ .$$

Assuming that $\eta(E) \propto E^{\alpha-1}$, where $\alpha \gg 1$, one obtains

$$p_i(\epsilon_i) \propto \left(1 - \frac{\epsilon_i}{E_b}\right)^{\alpha-1} \ . \tag{18}$$

Also, $\beta_{phys} = \frac{\alpha-1}{E_b}$. Let $q = \frac{\alpha-2}{\alpha-1}$. Then, $q < 1$, $\alpha - 1 = \frac{1}{1-q}$, and

$$p_i(\epsilon_i) \propto (1 - \beta_{phys}(1-q)\epsilon_i)^{\frac{1}{1-q}} \ ,$$

which is of the form given in (3).

By a simple refinement of the above argument, one can obtain the probability distribution of the form given in (4). The above expression for β_{phys} assumes that the heat bath always has energy E_b, irrespective of the energy of the system. However, the actual energy of the heat bath is $E_b - \epsilon_i$ when the system is in state i. Therefore, if the average energy of the system is U then the average energy of the heat bath is $E_b - U$. Hence, a more precise expression for β_{phys} is given by

$$\beta_{phys} = \frac{\alpha - 1}{E_b - U} \ .$$

Using this expression in (18), and with q defined as above, one obtains

$$p_i(\epsilon_i) \propto (1 - \beta_{phys}(1-q)(\epsilon_i - U))^{\frac{1}{1-q}} \ , \tag{19}$$

which is of the form given in (4). Requiring this distribution to be identical with (4) then gives

$$\beta_{phys} = \frac{\beta_3}{Y_3} \ ,$$

which is the same relation as in (17) and relates β_3 of the canonical ensemble approach to β_{phys}, the physical inverse temperature of the bath. Assuming

the validity of the argument of [8] and our refinement of it, the above relation is valid for any arbitrary system, but with $q < 1$.

8. We close with a few comments. The normalised q-expectation values have, indeed, been found earlier to possess desireable properties and, hence, considered to be the appropriate ones. Here, we find that this result follows simply by requiring the equivalence between the microcanonical and the canonical ensemble approaches.

However, we have considered here only systems whose $q = 1$ partition function is given by (5). Hence, it is desireable to establish this result for any arbitrary system whose $q = 1$ partition function is completely general.

The relation (16) between β_{mc} and β_{phys} is valid for any arbitrary system whose $q = 1$ partition function is completely general. The relation (17) between β_3 and β_{phys} is derived, in the first method, only for systems whose $q = 1$ partition function is given by (5). Assuming the validity of the argument of [8] and our refinement of it, the second method of derivation is valid for any arbitrary system, but with $q < 1$. Hence, a general relation between β_3 and β_{phys}, valid for any arbitrary system and for any value of q, is still lacking.

Also, Tsallis statistics is applied to a variety of diverse physical systems such as Levy flights, turbulence, etc. to name but a few [2, 3]. It is not clear if each one of them can be modelled as a system within a container, or as a system weakly interacting with a large, but finite, heat bath - models which played a crucial role in the physical interpretation of β_3 presented here. On the other hand, however, one may instead assume that $\frac{\beta_3}{Y_3}$, or a suitable generalisation of it, is indeed a physical quantity as given in (17). Its study may then, perhaps, provide new insights into physical systems, to which Tsallis statistics is applied.

Note: While this work was being written, a paper by Abe et al [10] has appeared. In the prescription termed *optimal Lagrange multipliers* formalism [11] which they use, the combination $\frac{\beta_3}{Y_3}$ appears naturally. As shown in [10], certain key properties of the ideal gas then become identical in both the standard statistical mechanics and Tsallis statistics.

The referee has brought to our attention a paper by Abe [12] where also the combination $\frac{\beta_3}{Y_3}$, termed *a renormalised (inverse) temperature*, appears naturally while establishing the zeroth law of thermodynamics using the clas-

sical ideal gas model.

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[9] The probability distributions in (3) and (4) are related by $\beta_2 = \beta_3\,(Y_3 + \beta_3(1-q)U_3)^{-1}$. Then $p_{i2} = p_{i3}$ and, therefore, $Y_3 = Y_2$, $U_3 = \frac{U_2}{Y_2}$, and $\beta_3 = \frac{\beta_2 Y_2^2}{Z_2^{1-q}}$. Other quantities such as free energy, specific heat, etc. can also be correspondingly related [5].

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